Extended X-ray Absorption Fine-structure Measurement of Bond-length Strain in Epitaxial Gd_2O_3 on GaAs(001)

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Beamline(s): **X23A2**

Introduction: We examine the microscopic structure of strained Gd_2O_3 films grown epitaxially on GaAs(001) using polarization-dependent extended x-ray absorption fine-structure (EXAFS).

Methods and Materials: The 23 Å thin Gd_2O_3 film was grown epitaxially on the GaAs(001) substrate wafer in an ultrahigh vacuum chamber at Bell Laboratories, Lucent Technologies. These films are single crystal, with a low number of defects and interfacial states, and they successfully have been used to create metal-oxide-semiconductor structures on GaAs (M. Hong et al., Science 283, 1897 (1999)).

EXAFS experiments were performed at the National Institute of Standards and Technology beamline X23-A2 at the NSLS. These samples are stable in air, as previously reported. The combined Gd $L\alpha_1$ and $L\alpha_2$ fluorescence yield around the Gd L_{III} edge ($h\nu$ = 7243 eV) was monitored using a single-element SiLi detector. EXAFS data were recorded with the sample surface normal **n** either parallel ($\boldsymbol{\varepsilon} \parallel \mathbf{n}$) or perpendicular ($\boldsymbol{\varepsilon} \perp \mathbf{n}$) to the polarization vector $\boldsymbol{\varepsilon}$ of the synchrotron radiation. In addition, EXAFS data from a pure Gd_2O_3 powder were collected in transmission, to determine the EXAFS phase and amplitude standards for the Gd-O bond length.

Results: Figure 1 shows the k^2-weighted Gd L_{III} edge EXAFS from the Gd_2O_3 powder. Also shown are the EXAFS from the Gd_2O_3 epitaxial film recorded in the two polarizations. The frequency of the EXAFS oscillations and therefore the Gd-O bond length r in the film is increased significantly relative to the powder. The best fits produce r = 2.391 ± 0.017 Å for $\boldsymbol{\varepsilon} \parallel \mathbf{n}$ and r = 2.389 ± 0.019 Å for $\boldsymbol{\varepsilon} \perp \mathbf{n}$, so together we determine an average Gd-O bond length r = 2.390 ± 0.013 Å. This is a +0.063 ± 0.013 Å or +2.7 ± 0.6 % increase relative to the 2.327 Å bond length in bulk Gd_2O_3.

In addition, the data from the two polarizations are identical within the noise throughout the entire k range. This indicates that the first and second shell local structures are similar along the [-110] and [110] directions of the strained Gd_2O_3 film; therefore, the strains along [-110] and [110] are equal, as suggested by the crystal symmetry of Gd_2O_3 .

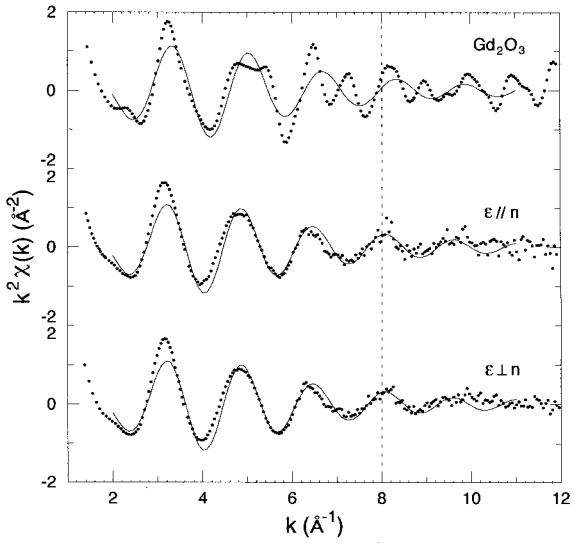

Fig. 1. k^2-weighted Gd L_{III} edge EXAFS from the Gd_2O_3 powder (top). Also shown are the EXAFS from the epitaxial Gd_2O_3 film on GaAs(001), as well as the best fits (solid lines) for the first-shell contribution. The data from the film were recorded with the polarization vector of the synchrotron radiation aligned parallel (middle, $\boldsymbol{\varepsilon} \parallel \mathbf{n}$) and perpendicular (bottom, $\boldsymbol{\varepsilon} \perp \mathbf{n}$) to the GaAs(001) surface normal. The frequency of the EXAFS oscillations and therefore the Gd-O bond length r in the film is increased significantly relative to the powder

Conclusions: Using a simple model with a unique Poisson distortion for the strained film that matches the [001] and [-110] axes of Gd_2O_3 with the [110] and [1-10] axes of the GaAs(001) surface, the measured bond-length increase of the film determined by EXAFS agrees well with the perpendicular lattice distortion of the film determined by diffraction (A.R. Kortan et al., Phys. Rev. B **60**, 10913).

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References: E. J. Nelson et al., Appl. Phys. Lett. **76,** 2526 (2000); M. Hong et al., Science **283**, 1897 (1999); A.R. Kortan et al., Phys. Rev. B **60**, 10913.

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